How an Anomalous Cusp Bifurcates

Robert S. Maier[1,2] and D. L. Stein[2,1]
[1]*Mathematics and* [2]*Physics Departments, University of Arizona, Tucson, Arizona 85721*

Abstract

We study the pattern of activated trajectories in a double well system without detailed balance, in the weak noise limit. The pattern may contain cusps and other singular features, which are similar to the caustics of geometrical optics. Their presence is reflected in the quasipotential of the system, much as phase transitions are reflected in the free energy of a thermodynamic system. By tuning system parameters, a cusp may be made to coincide with the saddle point. Such an anomalous cusp is analogous to a nonclassical critical point. We derive a scaling law, and nonpolynomial 'equations of state', that govern its bifurcation into conventional cusps.

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The *optimal trajectory* concept has been widely used in the theory of noise-activated transitions [1–7]. In the weak noise limit, when transitions between stable states become exponentially rare, one or at most a few trajectories in the system state space are singled out as escape paths of least resistance. Also, between the energetically lowest stable state and any other state there are at most a few dominant activated trajectories. Such optimal trajectories, which are determined by a 'least energy expended' or 'least action' variational principle, are experimentally observable [6,7]. In systems that have the property of detailed balance, they are time-reversed relaxational trajectories. But in nonequilibrium systems, which lack detailed balance, the optimal trajectory pattern extending from a stable state may be more complicated.

Optimal trajectories are similar in many ways to the rays of geometrical optics, which characterize in the short wavelength limit the waves emanating from a point source. That is because optical rays may be computed variationally too, from a 'least optical depth' principle. In a medium with inhomogeneous index of refraction, it is common for a ray family to bounce off a *caustic surface*, leaving the region behind in shadow: not illuminated, or illuminated only indirectly. Other singular features with a catastrophe-theoretic interpretation may be produced [8,9]. In a noise-driven system in which detailed balance is violated, the pattern of optimal trajectories may contain similar features [1,5,10]. See Fig. 1.

To understand the crossing of optimal trajectories, it is useful to look at the *quasipotential* of the noise-driven system. If ϵ is the noise strength (e.g., $\epsilon = kT$ in thermal systems), and $\rho(\mathbf{x})$ denotes the stationary probability density of the system at state $\mathbf{x}$, then a quasipotential $W = W(\mathbf{x})$ may be defined phenomenologically by

$$\rho(\mathbf{x}) \sim \text{const} \times \exp[-W(\mathbf{x})/\epsilon], \qquad \epsilon \to 0. \tag{1}$$

This definition makes sense whether or not the system dynamics are conservative, and whether or not the noise acts so as to preserve detailed balance. W equals zero at the energetically lowest stable state(s), and $W(\mathbf{x})$ is essentially the minimum energy needed to excite the system to state $\mathbf{x}$. It may be computed as a line integral along the optimal trajectory extending to $\mathbf{x}$.

Formally, W is multivalued at any state, such as the states near a caustic, that is reached by more than one optimal trajectory emanating from the energetically lowest state(s). But by (1), the least value is dominant, and the trajectories giving rise to others are unphysical. The state space of a noise-driven system is typically partitioned by 'switching surfaces', on which dominance switches between branches of W.

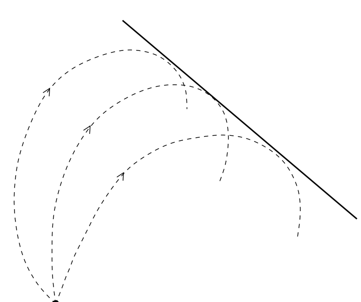

FIG. 1. How a caustic (solid curve) could be formed as the envelope of a family of outgoing optimal trajectories.

The switching of dominance resembles a first-order phase transition in a condensed matter system. The similarity is unsurprising, since phase transitions with classical critical exponents also have a catastrophe-theoretic interpretation [9]. Consider, for example, a ferromagnetic system with extensive order parameter m (magnetization), in a magnetic field h. Its thermodynamics are determined by a free energy function $\Psi = \Psi(T, h)$. Below the critical temperature T_c, Ψ and $m = \partial\Psi/\partial h$ are multivalued. If the phase transition is classical, i.e., of mean-field form, Ψ is three-valued in a sharp-tipped region of the (T, h) plane bounded by 'spinodals' of the form $h \approx \pm\text{const} \times (T_c - T)^{3/2}$. That is because the leading terms in the Legendre transform $\widetilde{\Psi}^{(h)}(T, m) \equiv hm - \Psi(T, h)$ are of Ginzburg–Landau type:

$$\widetilde{\Psi}^{(h)}(T, m) \approx C_2(T - T_c)m^2/2 + C_4 m^4/4. \tag{2}$$

In the catastrophe-theoretic sense [8,9], the spinodals are *fold caustics*. Each is the projection of a fold in the graph of Ψ, which is a two-dimensional surface, onto the (T, h) plane. The critical point $(T_c, 0)$ from which the spinodals extend is a *cusp catastrophe*: the projection of the point on the graph of Ψ at which the two folds join. A first-order phase transition line, on which dominance switches between branches of Ψ, extends from $(0, 0)$ to $(T_c, 0)$.

Switching lines in two-dimensional noise-driven systems are clearly analogous to first-order phase transition lines, and caustics to spinodals. Caustics typically terminate at cusps, and switching lines also frequently terminate at cusps. So cusps, which are very common, are analogous to second-order critical points [2]. They are physically important because at any cusp, the prefactor 'const' in (1), which in general is $\mathbf{x}$-dependent, diverges.

In previous work [1,2], we pointed out that in many noise-driven two-dimensional double well systems without detailed balance, a cusp may be moved to coincide with the saddle point between the wells, by tuning parameters. If they coincide, the Kramers ($\epsilon \to 0$) limit of noise-induced interwell transitions is greatly affected. The prefactor in the Kramers transition rate formula becomes anomalous: it acquires a negative power of ϵ.

Precisely at criticality, we were able to approximate the quasipotential W near any such 'anomalous cusp'. Our expression differed from the polynomial 'normal forms' of conventional catastrophe theory. In thermodynamics, it would correspond to a *nonclassical* phase transition. In catastrophe theory, it would be interpreted as a *nongeneric* catastrophe: one of the few such of physical relevance to have been discovered since the work of Berry and Mount on the short wavelength limit of scattering [8].

In this Letter, we extend Ref. [2] by analysing the 'unfolding' of an anomalous cusp in a typical two-dimensional noise-activated system, as a parameter is moved toward or away from criticality. We explain how it may bifurcate into conventional cusps. Our scaling law for the bifurcation yields a corresponding law for the divergence of the Kramers prefactor [11].

Consider the following double well model, which is similar to models of blocking dynamics in glassy systems, where a particle is coupled to a randomly fluctuating barrier whose position is coupled to the particle motion [12]. Let x (a particle position variable) and y (a barrier state variable) be nontrivially coupled in such a way that the values ±1 for x and 0 for y are stable. If x and y are overdamped and are driven by white noise of strength ϵ, their joint dynamics could be modeled by Langevin equations

$$\begin{aligned}\dot{x} &= \lambda_x \left[x\left(1 - x^2\right) - \alpha x y^2\right] + \epsilon^{1/2}\eta_x(t) \\ \dot{y} &= -|\lambda_y|(1 + x^2)y + \epsilon^{1/2}\eta_y(t).\end{aligned} \tag{3}$$

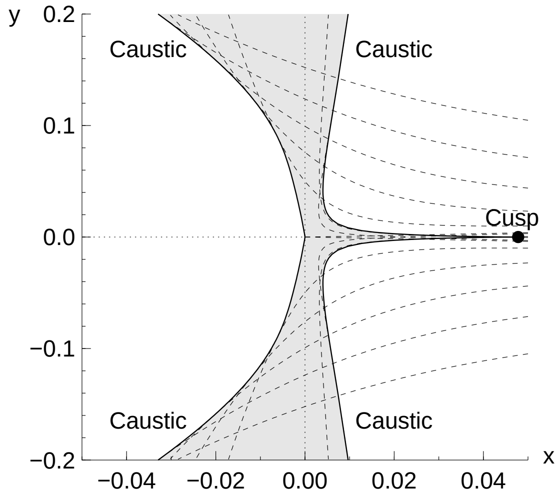

FIG. 2. The pattern of optimal trajectories near the saddle, in the 'broken phase' ($\alpha > \alpha_c$). Here $\lambda_x = 1$, $|\lambda_y| = 1.1$, $\alpha = 4.64$, and the critical value α_c equals 4.62. In the shaded region the quasipotential W is multivalued, and a switching line extends from $(0, 0)$ to the cusp $(x_c, 0) \approx (0.048, 0)$.

The parameters $\lambda_x > 0$ and $\lambda_y < 0$ determine the time scales on which x and y evolve, and govern the all-important relaxational behavior near the saddle point $(0, 0)$, where $(\dot{x}, \dot{y}) \approx (\lambda_x x, -|\lambda_y| y)$. The forcing terms (η_x, η_y) are a pair of independent Gaussian white noises, so that $\langle \eta_i(s)\eta_j(t)\rangle$ equals $\delta_{ij}\delta(s - t)$. The parameter α controls the absence of detailed balance: only when α equals $\mu \equiv |\lambda_y|/\lambda_x$ is there detailed balance, since only in that case is the drift field derived from a potential.

Our results are insensitive to the details of the coupling between x and y, so long as the model is symmetric through $x = 0$ and $y = 0$. To compute the pattern of optimal trajectories emanating from the bottom of the $x < 0$ well or the $x > 0$ well, we use the fact that in any multidimensional noise-driven system with vector Langevin equation $\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}) + \epsilon^{1/2}\boldsymbol{\eta}(t)$, the optimal trajectories are really zero-energy *Hamiltonian* trajectories, generated by the Wentzell–Freidlin Hamiltonian [13]

$$H(\mathbf{x}, \mathbf{p}) = \mathbf{p}^2/2 + \mathbf{u}(\mathbf{x}) \cdot \mathbf{p}. \tag{4}$$

That is because the associated Hamilton's principle is

$$\delta \int L(\mathbf{x}, \dot{\mathbf{x}})\, dt = \delta \int |\dot{\mathbf{x}} - \mathbf{u}(\mathbf{x})|^2\, dt = 0,$$

which is clearly a 'least energy expended' principle. The conjugate momentum $\mathbf{p} \equiv \partial L/\partial \dot{\mathbf{x}}$ equals $\dot{\mathbf{x}} - \mathbf{u}$, which measures the system's motion against the drift.

Figure 2 was obtained from (3) and (4) by integrating Hamilton's equations outward, at zero energy, from $(1, 0)$, i.e., from the bottom of the right-hand well. A small portion of the $x < 0$ half-plane is reached by optimal trajectories, but the rest is in shadow. In phase space, which is four-dimensional, the optimal trajectories trace out a two-dimensional manifold, called a Lagrangian manifold. This manifold lies 'above' only a small part of the $x < 0$ half-plane. It folds over, covering the shaded portion of the (x, y) plane more than once.

In the shaded region, the momentum $\mathbf{p}$ and the quasipotential W, which equals $\int \mathbf{p}\cdot d\mathbf{x}$, are two-valued ($x < 0$) or three-valued ($x > 0$). At any point $\mathbf{x}$, $\mathbf{p}$ equals $\boldsymbol{\nabla} W(\mathbf{x})$.

In Fig. 2, the parameter α is chosen to be slightly greater than a certain critical value, α_c. If there is detailed balance, the optimal trajectory pattern contains no singular features, but if α is increased through α_c, a cusp $(x_c, 0)$ emerges from the saddle point at $(0, 0)$ and moves toward $(1, 0)$. This phenomenon is not peculiar to the model defined by (3). In any symmetric two-dimensional double well system that violates detailed balance and has a tunable parameter, a similar cusp may be born. The focusing of optimal trajectories at the cusp resembles the focusing of rays in a radially symmetric optical system.

The value α_c can be computed from the second-order variational equation $\delta^2 \int L\, dt = 0$, which is a criterion for bifurcation. On physical grounds, when $\alpha < \alpha_c$, $\delta^2 \int L\, dt$ computed along the on-axis trajectory to the saddle is positive, but when $\alpha > \alpha_c$, it is negative. In the model (3), α_c turns out (cf. Ref. [2]) to equal $2\mu(\mu + 1)$.

The cusp $(x_c, 0)$ that is present when $\alpha > \alpha_c$ resembles a second-order critical point. W is three-valued in the sharp-tipped region extending from it, which is bounded by 'spinodals' of the form $y \approx \pm\mathrm{const} \times (x_c - x)^{3/2}$. (See Fig. 2.) Moreover, there is a switching line extending from the saddle at $(0, 0)$ to $(x_c, 0)$. As noted, this line is analogous to a first-order phase transition line.

What remains to be understood is how the cusp is born at $\alpha = \alpha_c$. In a three-dimensional space with coordinates $(x, y; \alpha)$, there is a line of second-order critical points in the $y = 0$ plane that extends from $(0, 0; \alpha_c)$ to $(1, 0; +\infty)$. By analogy with thermodynamics, one might expect $(0, 0; \alpha_c)$ to be a third-order critical point. At any fixed $\alpha > \alpha_c$, the leading terms in the Legendre transform $\widetilde{W}^{(y)}(x, p_y) \equiv yp_y - W$, close to the cusp, are known to be of Ginzburg–Landau type [2,5]:

$$\widetilde{W}^{(y)}(x, p_y) \approx C_2(\alpha)[x - x_c(\alpha)]p_y^2/2 + C_4(\alpha)p_y^4/4. \tag{5}$$

One might expect that the correct three-dimensional generalization would be a higher-degree polynomial in x, p_y, and $\alpha - \alpha_c$. That would allow the birth of the cusp to be viewed as a classical phase transition, or one of the generic (polynomial) elementary catastrophes [8,9].

In Ref. [2] we presented initial evidence against this. At criticality ($\alpha = \alpha_c$), we were able to construct a scaling solution for W, valid near the x-axis close to the saddle. The equation satisfied by the scaling function contained non-integer powers: in fact, powers that depended continuously on the model parameter μ.

By linearizing Hamiltonian dynamics near the saddle, we have now characterized fully the behavior of the quasipotential W near a singular point like $(0, 0; \alpha_c)$. Our chief new result is a *cubic equation* satisfied by the double Legendre transform of W. It defines a higher-order, but nonclassical, critical point. We have also extended our $\alpha = \alpha_c$ scaling law to the case when $|\alpha - \alpha_c|$ is nonzero but small. These results should extend to any symmetric double well system with a tunable parameter.

Figure 3, which was obtained in the 'unbroken phase' ($\alpha < \alpha_c$), sheds light on behavior near criticality. The crucial feature is the two caustics, relics of which appeared in Fig. 2. They form part of the boundary of the 'illuminated' region. Each caustic extends from a cusp, which is located very close to the y-axis separatrix between the two wells. As $\alpha \to {\alpha_c}^-$, the cusps *neck down* to the saddle. Any further increase in α causes the x-axis cusp to be born, and to move toward positive x.

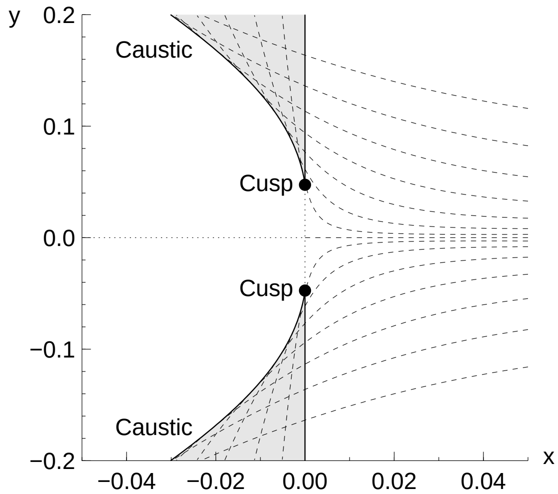

FIG. 3. The pattern of optimal trajectories near the saddle, in the 'unbroken phase' ($\alpha < \alpha_c$). Here $\lambda_x = 1$, $|\lambda_y| = 1.1$, $\alpha = 4.61$, and the critical value α_c equals 4.62. As $\alpha \to {\alpha_c}^-$, the two cusps close to the y-axis neck down to the saddle.

The merged cusp at $(0,0)$, when $\alpha = \alpha_c$, is truly anomalous. It is the projection of a point on the boundary of the Lagrangian manifold, rather than of a point in its interior. So it is a *boundary catastrophe*: a singular point of a sensitive kind. To explain its bifurcation into cusps on the x-axis or y-axis, we must approximate the optimal trajectory pattern in a neighborhood of the saddle, for $|\alpha - \alpha_c|$ nonzero but small.

We accordingly linearize Hamilton's equations, which any optimal trajectory must satisfy, near the point $(x, y; p_x, p_y) = (0, 0; 0, 0)$ in phase space. A simple analysis (cf. Ref. [3]) shows that this fixed point has two stable directions, $\mathbf{e}_s = (0, 1; 0, 0)$ and $\tilde{\mathbf{e}}_s = (1, 0; -2\lambda_x, 0)$, and two unstable directions, $\mathbf{e}_u = (1, 0; 0, 0)$ and $\tilde{\mathbf{e}}_u = (0, 1; 0, 2|\lambda_y|)$. The zero-momentum directions (no tilde) are eigendirections for relaxational trajectories, which follow the drift. In the linear approximation, any optimal trajectory near $(x, y) = (0, 0)$ must satisfy

$$\begin{aligned}(x, y; p_x, p_y) \approx\ & C_s e^{-|\lambda_y|t}\mathbf{e}_s + \widetilde{C}_s e^{-\lambda_x t}\tilde{\mathbf{e}}_s \\ & + C_u e^{\lambda_x t}\mathbf{e}_u + \widetilde{C}_u e^{|\lambda_y|t}\tilde{\mathbf{e}}_u\ ,\end{aligned} \tag{6}$$

where the C's are trajectory-specific constants.

We now index the 'fan' of optimal trajectories that approach the saddle point, as in Figs. 2 and 3, by s. The normalization of this index variable is somewhat arbitrary. A reasonable choice would be for it to denote distance from the x-axis (at a fixed $x > 0$, near the saddle). With this choice, $s = 0$ will correspond to the uphill optimal trajectory that climbs toward $(0,0)$ along the positive x-axis. If each coefficient in (6) can be expanded in s about $s = 0$, then by symmetry considerations

$$C_s = a_1 s + a_3 s^3 + \cdots, \tag{7a}$$
$$\widetilde{C}_s = b_0 + b_2 s^2 + \cdots, \tag{7b}$$
$$C_u = c_2 s^2 + c_4 s^4 + \cdots, \tag{7c}$$
$$\widetilde{C}_u = d_1 s + d_3 s^3 + \cdots. \tag{7d}$$

We identify the passage through criticality, as α is increased through α_c, with the passing through zero of the coefficients c_2 and d_1. So, setting $\delta \equiv \alpha_c - \alpha$, we take c_2 and d_1 to be linearly proportional to δ, to leading order.

Eq. (6) comprises four scalar equations. Eliminating s and t among them, we can derive 'equations of state' relating δ and any three of the phase space coordinates x, y, p_x, and p_y. When $|\delta| \ll 1$, the equation relating x, y, p_y, and δ (near the x-axis), and the equation relating x, y, p_x, and δ (near the y-axis), turn out to be, respectively,

$$0 = (p_y - 2|\lambda_y|y)^3 + k_1\delta x^{2\mu}(p_y - 2|\lambda_y|y) + k_0 x^{4\mu} p_y \tag{8a}$$

$$0 = (p_x + 2\lambda_x x)^3 + \ell_1\delta p_x^{2\mu-2} y^2 (p_x + 2\lambda_x x) + \ell_0 y^4 p_x^{4\mu-3} \tag{8b}$$

Here k_1, k_0, ℓ_1, and ℓ_0 are positive constants. At criticality ($\delta = 0$), (8a)–(8b) reduce to the equations we previously obtained by an altogether different technique [2].

By definition, the cusp $(x_c, 0)$ is the point on the positive x-axis where W or $(p_x, p_y) = \boldsymbol{\nabla} W$ stops being multivalued as a function of (x, y), as x increases from 0. It is easy to verify from (8a) that when δ is small and negative (i.e., $\alpha - \alpha_c$ is small and positive), the cusp location x_c satisfies $x_c \propto (-\delta)^{1/2\mu}$. The δ-dependence of the parent cusps, which have $y = \pm y_c$, can be computed from (8b). They are the points close to the y-axis where (p_x, p_y) first becomes multivalued, as $|y|$ increases from zero. When $\delta \to 0^+$ (i.e., $\alpha \to {\alpha_c}^-$), we find that the parent cusps neck down at the rate $y_c \propto \delta^{3/2-\mu}$. That is so when $1 \le \mu < 3/2$, at least; for other μ, the prediction is that there are no parent cusps, and no necking down. All these predictions have been numerically confirmed [11].

Despite the continuously varying exponents, the emergence of the x-axis cusp is surprisingly similar to a second-order phase transition. Recall that close to the ferromagnetic critical point defined by (2), scaled magnetization M and scaled magnetic field H are related by

$$M^3 \pm M - H = 0, \tag{9}$$

or equivalently by the scaling law $M = \phi_\pm(H)$. Here $M \equiv Am/|T - T_c|^{1/2}$ and $H \equiv Bh/|T - T_c|^{3/2}$, with $A \equiv \sqrt{C_4/C_2}$ and $B \equiv A^3/C_4$. The plus (minus) applies when $T - T_c$ is positive (negative). Eq. (8a) may be rewritten in the form (9), provided that one defines

$$M \equiv (p_y - 2|\lambda_y|y)/|k_1\delta x^{2\mu} + k_0 x^{4\mu}|^{1/2} \tag{10}$$

$$H \equiv 2|\lambda_y| k_0 x^{4\mu} y/|k_1\delta x^{2\mu} + k_0 x^{4\mu}|^{3/2}. \tag{11}$$

The plus (minus) applies when $k_1\delta x^{2\mu} + k_0 x^{4\mu}$ is positive (negative). The law $M = \phi_\pm(H)$, in which δ appears implicitly, provides a unified description of the x-axis behavior both at criticality ($\delta = 0$) and away ($\delta \ne 0$).

The most striking consequence of this approach is a general scaling law, showing how the quasipotential varies as $(x, y; \alpha)$ moves away from $(0, 0; \alpha_c)$, *in any direction*. It can be written using the double Legendre transform $\widetilde{W}^{(x,y)}(p_x, p_y) \equiv \mathbf{x} \cdot \mathbf{p} - W$, which equals $\int \mathbf{x} \cdot d\mathbf{p}$. Near the saddle,

$$W(x,y) \approx W(0,0) - \lambda_x x^2 + |\lambda_y| y^2 \tag{12}$$

$$\widetilde{W}^{(x,y)}(p_x,p_y) \approx -W(0,0) - p_x^2/4\lambda_x + p_y^2/4|\lambda_y|. \tag{13}$$

Let $R = R(p_x,p_y)$ denote the difference between $\widetilde{W}^{(x,y)}$ and the right-hand side of (13). Since $\widetilde{W}^{(x,y)} = \int \mathbf{x}\cdot\dot{\mathbf{p}}\,dt$, R may be expressed in terms of s and t by employing (6) and (7). By eliminating s and t from the formulæ for $R(s,t)$, $p_x(s,t)$, and $p_y(s,t)$, we find to leading order in δ

$$R^3 + m_1 \delta p_x^{2\mu} p_y^2 R - m_0 p_x^{4\mu} p_y^4 = 0, \tag{14}$$

where m_1 and m_0 are positive constants. This is the extension to $\delta \neq 0$ of a formula derived in Ref. [2].

In phase transition language, the cubic equation (14) fully characterizes the nonclassical structure of the critical point $(x,y;\alpha) = (0,0;\alpha_c)$, i.e., $(p_x,p_y;\alpha) = (0,0;\alpha_c)$. Equation (14) is also interesting from a catastrophe theory point of view. Nongeneric catastrophes, which are difficult to classify, may in general be perturbed in an infinite number of ways so as to yield generic catastrophes [8]. But (14) describes the bifurcation of a nongeneric catastrophe (the anomalous cusp) into conventional cusps, in a unique, physically determined way.

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